

Sucralose

56038-13-2 | DTXSID1040245

Model Performance

Model

Data

Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.89	0.25	0.88	0.26	0.75	0.38

Model Results

Predicted value: 4.35 days

Global applicability domain: Outside

Local applicability domain index: 2.77e-01

Confidence level: 8.75e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>1-Methyl-2-propylbenzene</div> <div>Measured: 3.00</div> <div>Predicted: 3.17</div>	<div>Image not found</div> <div>5-Methylindan</div> <div>Measured: 2.00</div> <div>Predicted: 2.25</div>	<div>Image not found</div> <div>9-Ethyl-9H-fluorene</div> <div>Measured: 29.0</div> <div>Predicted: N/A</div>
<div>Image not found</div> <div>3-Ethyltoluene</div> <div>Measured: 3.00</div> <div>Predicted: 3.26</div>	<div>Image not found</div> <div>1H-Indene, 2-methyl-</div> <div>Measured: 3.00</div> <div>Predicted: 2.48</div>	